Uncertainty Analysis for Complex Systems: Algorithms for Practical Systems

Dongbin Xiu

Department of Mathematics, Purdue University

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Overview

- Stochastic PDE: Re-formulation

- Solution Strategies: generalized polynomial chaos (gPC)

- Application: Epistemic uncertainty analysis

(Re-)Formulation of PDE: Input Parameterization

$$\frac{\partial u}{\partial t}(t,x) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Goal:** To characterize the random inputs by a set of random variables
  - Finite number
  - Mutual independence

- **If inputs == parameters**
  - Identify the (smallest) independent set
  - Prescribe probability distribution
- **Else if inputs == fields/processes**
  - Approximate the field by a function of finite number of RVs
  - Well-studied for Gaussian processes
  - Under-developed for non-Gaussian processes
  - Examples: Karhunen-Loeve expansion, spectral decomposition, etc.

$$a(x,\omega) \approx \mu_a(x) + \sum_{i=1}^{d} \tilde{a}_i(x) Z_i(\omega)$$

The Reformulation

- **Stochastic PDE:**

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Solution:** $u(t,x,Z) : [0,T] \times \bar{D} \times \mathbb{R}^{n_z} \to \mathbb{R}$

- Uncertain inputs are characterized by n_z random variables Z

- Probability distribution of Z is prescribed

$$F_Z(s) = \Pr(Z \leq s), \quad s \in \mathbb{R}^{n_z}$$

Non-trivial task

Generalized Polynomial Chaos (gPC)

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Focus on dependence on *Z*:** $u(\bullet, Z) : \mathbb{R}^{n_Z} \to \mathbb{R}$

- ***N*th-order gPC expansion:**

$$u_N(t,x,Z) \triangleq \sum_{|\mathbf{k}|=0}^{N} \hat{u}_{\mathbf{k}}(t,x)\Phi_{\mathbf{k}}(Z), \quad \#\text{ of basis} = \begin{pmatrix} n_z + N \\ N \end{pmatrix}$$

- **Orthogonal basis:** $\int \Phi_{\mathbf{i}}(Z)\Phi_{\mathbf{j}}(Z)\rho(Z)\,dZ = \delta_{\mathbf{ij}}$

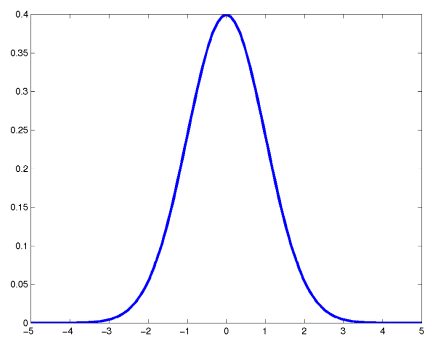
- **Basis functions:**
  - Hermite polynomials: seminal work by *R. Ghanem*
  - General orthogonal polynomials *(Xiu & Karniadakis, 2002)*

- **Properties:**
  - Rigorous mathematics
  - High accuracy, fast convergence
  - Curse-of-dimensionality
- **Numerical Approaches:**
  - Galerkin vs. collocation

gPC Basis

- **Expectation:** $$\mathbb{E}\big(g(Z)\big) = \int_{\mathbb{R}} g(z)\rho(z)\,dz$$

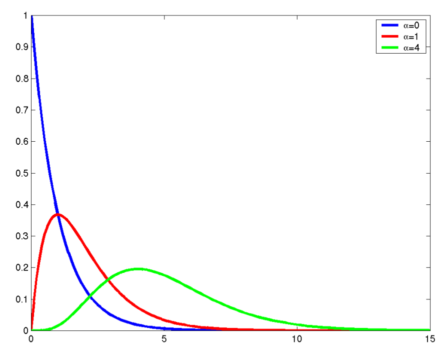
- **Orthogonality:** $$\int \Phi_{\mathrm{i}}(z)\Phi_{\mathrm{j}}(z)\rho(z)\,dz = \mathbb{E}\big[\Phi_{\mathrm{i}}(Z)\Phi_{\mathrm{j}}(Z)\big] = \delta_{\mathrm{ij}}$$



Gaussian distribution

$$\int_{-\infty}^{\infty} \Phi_{\mathrm{i}}(z)\Phi_{\mathrm{j}}(z)e^{-z^2}\,dz = \delta_{\mathrm{ij}}$$

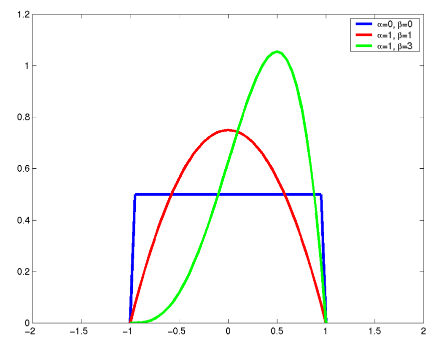
Hermite polynomial



Gamma distribution

$$\int_{0}^{\infty} \Phi_{\mathrm{i}}(z)\Phi_{\mathrm{j}}(z)e^{-z}\,dz = \delta_{\mathrm{ij}}$$

Laguerre polynomial



Beta distribution

$$\int_{-1}^{1} \Phi_{\mathrm{i}}(z)\Phi_{\mathrm{j}}(z)\,dz = \delta_{\mathrm{ij}}$$

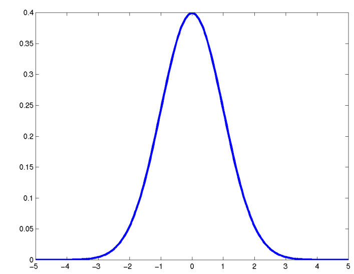
Legendre polynomial

gPC Basis: the Choices

- **Orthogonality:** $$\int \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)\rho(z)\,dz = \mathbb{E}\left[\Phi_{\mathbf{i}}(Z)\Phi_{\mathbf{j}}(Z)\right] = \delta_{\mathbf{ij}}$$

- **Example: Hermite polynomial**

$$\int_{-\infty}^{\infty} \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)e^{-z^2}\,dz = \delta_{\mathbf{ij}}$$

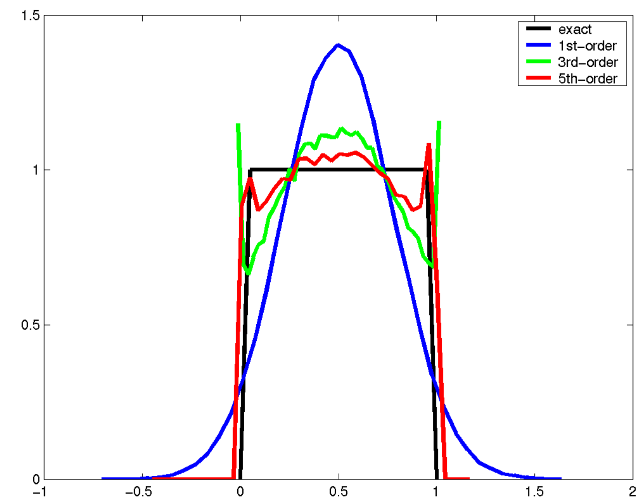


- **The polynomials:** *Z~N(0,1)*

$$\Phi_0 = 1, \quad \Phi_1 = Z, \quad \Phi_2 = Z^2 - 1, \quad \Phi_3 = Z^3 - 3Z, \quad \cdots$$

- **Approximation of arbitrary random variable:** Requires L^2 integrability

- **Example:** Uniform random variable
  - Convergence
  - Non-optimal
  - First-order Legendre is exact

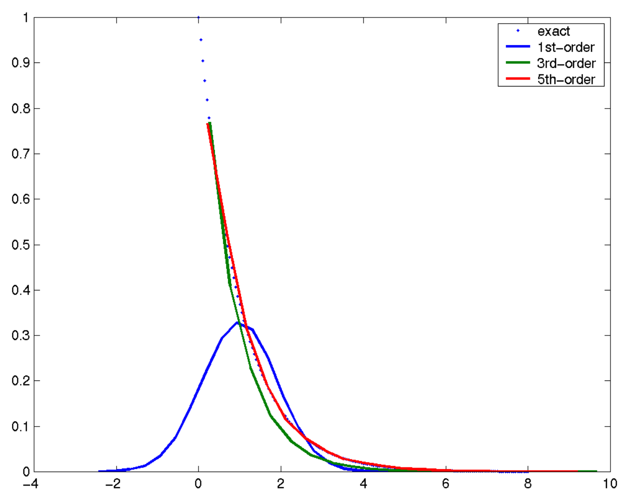


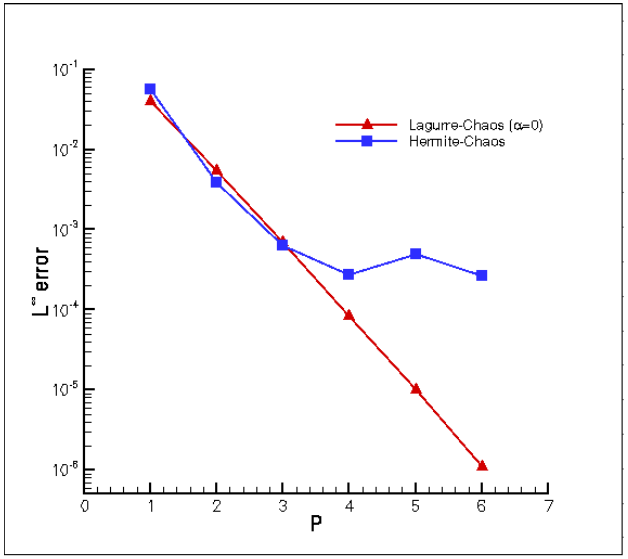
Computational Efficiency

- First-order ODE: exponential random input

Error	**Monte Carlo Method** (# of realizations)	**Generalized Polynomial Chaos** (# of expansion terms)	**Speed-up factor**
4%	100	1	100
1.1%	1,000	2	500
0.05%	9,800	3	3,267

Effect of non-optimal basis





Stochastic Galerkin

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Galerkin method:** Seek

$$u_N(t,x,Z) \triangleq \sum_{|\mathbf{k}|=0}^{N} \hat{u}_{\mathbf{k}}(t,x)\Phi_{\mathbf{k}}(Z)$$

Such that

$$\mathbb{E}\left[\frac{\partial u_N}{\partial t}(t,x,Z)\mathbf{\Phi}_{\mathbf{m}}(Z)\right] = \mathbb{E}\left[\mathcal{L}(u_N)\mathbf{\Phi}_{\mathbf{m}}(Z)\right], \quad \forall|\mathbf{m}| \le N$$

- **The result:**
  - Residue is orthogonal to the gPC space
  - A set of deterministic equations for the coefficients
  - The equations are usually coupled – requires new solver

Stochastic Collocation

$$\frac{\partial u}{\partial t}(t, x, Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Collocation:** To satisfy governing equations at selected nodes
  - Allow one to use existing deterministic codes repetitively

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- **Sampling:** (solution statistics only)
  - Random (Monte Carlo)
  - Deterministic (lattice rule, tensor grid, cubature)

- **Stochastic collocation:** To construct **polynomial approximations**
  - Node selection is critical to efficiency and accuracy
  - More than sampling

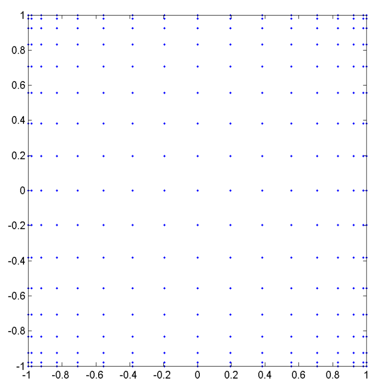
Stochastic Collocation: Interpolation

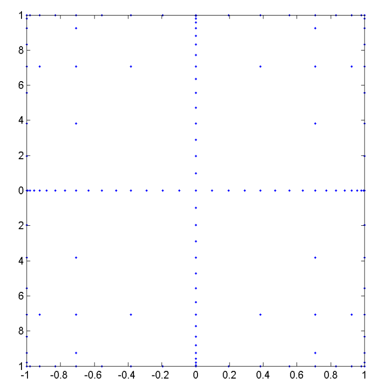
$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Definition:** Given a set of nodes and solution ensemble, find u_N in a proper polynomial space, such that $u_N \approx u$ in a proper sense.

- **Interpolation Approaches:** $$u_N(Z) = \sum_{j=1}^{Q} u(Z^j) L_j(Z)$$ $$L_i(Z^j) = \delta_{ij}, \quad 1 \le i, j \le Q$$

  - Dimension-by-dimension space filling





Tensor grids: inefficient

Sparse grids: more efficient

(Xiu & Hesthaven, SIAM J. Sci. Comput., 05)

Stochastic Computation: The Landscape

- **Realistic Large-scale Complex Systems:**
  - Complex physics ➔ highly nonlinear systems
  - Large number of random variables
  - (Extremely) time consuming simulations
  - Legacy codes (nearly impossible to re-write)

- **Stochastic Galerkin:**
  - Difficult to implement
  - Good mathematical properties

- **Stochastic collocation is more proper:**
  - Easy to implement ➔ virtually no coding effort
  - Nonlinearity poses no additional difficulties

Epistemic Uncertainty: Setup

- **Governing Equation:**

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x,Z) = \mathcal{L}(v), & D \times (0,T] \times I_Z \\ \mathcal{B}(v) = 0, & \partial D \times [0,T] \times I_Z \\ v = v_0, & D \times \{t = 0\} \times I_Z \end{cases}$$

$$v(x,t,Z) : \bar{D} \times [0,T] \times I_Z \to \mathbb{R} \qquad I_Z \subseteq \mathbb{R}^d$$

- **Epistemic uncertainty:**
  - Distribution of Z is not fully known

- **"Some" prior knowledge:**

$$I_{Z_i} = [\alpha_i, \beta_i], \quad -\infty \leq \alpha_i < \beta_i \leq \infty$$

$$I_Z \subseteq \bigtimes_{i=1}^{d} I_{Z_i}$$

- **Remark:** Z_i can be dependent, unbounded, and I_Z can be much smaller.

Encapsulation

- **Goal: To "encapsulate" each variable**
  - For each Z_i (potentially unbounded), find a bounded interval to "capture" it.
  - Requires modeling effort

- **Overwhelming probability condition:**

For each $I_{Z_i} = [\alpha_i, \beta_i], \quad \alpha_i < \beta_i,$ find a bounded interval

$$I_{X_i} = [a_i, b_i], \quad -\infty < a_i < b_i < \infty,$$

such that

$$\Pr(Z_i \in I_i^-) \le \delta_i,$$

where $\delta_i \ge 0,$ and I_i^- is the difference set

$$I_i^- = I_{Z_i} \, \Delta \, I_{X_i} = \left(I_{Z_i} \cup I_{X_i}\right) \backslash \left(I_{Z_i} \cap I_{X_i}\right)$$

- If Z_i is bounded, it is "easier" to do
- If Z_i is unbounded, X_i needs to be "big" enough

Encapsulation (cont'd)

- For each variable:

$$I_{Z_i} = [\alpha_i, \beta_i], \quad -\infty \le \alpha_i < \beta_i \le \infty$$

$$I_{X_i} = [a_i, b_i], \quad -\infty < a_i < b_i < \infty$$

$$\Pr(Z_i \in I_i^-) \le \delta_i$$

- For all variables:

$$I_Z \subseteq \mathop{\times}_{i=1}^{d} I_{Z_i}$$

$$\boxed{I_X = \mathop{\times}_{i=1}^{d} I_{X_i} = \mathop{\times}_{i=1}^{d} [a_i, b_i]}$$

$$I^+ = I_Z \cup I_X, \qquad I^o = I_Z \cap I_X$$

$$I^- = I_Z \,\Delta\, I_X = I^+ \setminus I^o \ \text{(difference set)}$$

- Overwhelming probability condition:

$$\Pr(Z_i \in I^-) \le \delta, \qquad \delta = 1 - (1 - \delta_i)^d$$

- Reminder: I_X may not overlap I_Z

Encapsulation Problem

- **Original Problem:**

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x,Z) = \mathcal{L}(v), & D\times(0,T]\times I_Z \\ \mathcal{B}(v)=0, & \partial D\times[0,T]\times I_Z \\ v = v_0, & D\times\{t=0\}\times I_Z \end{cases}$$

- **Encapsulation Problem:**

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x,X) = \mathcal{L}(u), & D\times(0,T]\times I_X \\ \mathcal{B}(u)=0, & \partial D\times[0,T]\times I_X \\ u = v_0, & D\times\{t=0\}\times I_X \end{cases}$$

  - Solution in a hypercube: $u(x,t,X): \bar{D}\times[0,T]\times I_X \to \mathbb{R}$

$$I_X = [a_i, b_i]^d \,(= [-1,1]^d, = [0,1]^d)$$

- **Assumption:** $u(\cdot,\xi) = v(\cdot,\xi), \quad \forall \xi \in I^o$

Solution Strategy of the Encapsulation Problem

- **Encapsulation Problem:**

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x,X) = \mathcal{L}(u), & D\times(0,T]\times I_X \\ \mathcal{B}(u) = 0, & \partial D\times[0,T]\times I_X \\ u = v_0, & D\times\{t=0\}\times I_X \end{cases}$$

- **Solution strategy: Controllability on point-wise error**

$$\varepsilon_n = \left\| u - u_n \right\|_{L^\infty(I_X)} \to 0, \qquad n\to\infty$$

  - u_n is a good approximation in the entire domain I_X (hypercube)
  - Can "sample" u_n accurately for all realizations
  - No probability distribution is assigned in I_X.
  - Convergence is a mathematical preference, not a practical necessity

- Requirement on error control is strong but achievable
  - Sparse grid collocation (with sufficient regularity)
  - Polynomial Galerkin (e.g., Chebyshev) methods are possible
  - Without sufficient regularity --- multi-element approach

Solution "Statistics"

- Solution of the original problem:

$$v(\cdot, Z) : I_Z \to \mathbb{R} \qquad \mu = \int_{I_Z} v(s)\rho_Z(s)ds$$

- Solution in the hypercube: $I^o = I_Z \cap I_X$

$$u_n(\cdot, X) : I_X \to \mathbb{R} \qquad \mu_n = \int_{I^o} u_n(s)\rho_Z(s)ds$$

Theorem: Assume $v(Z)$ is bounded and let $C_v = \|v\|_{L^\infty(I_Z)}$. Let u_n be an approximation to the solution of the encapsulation problem $u(X)$, s.t.,

$$\varepsilon_n = \|u - u_n\|_{L^\infty(I_X)}.$$

Then the approximation of the mean solution satisfies

$$|\mu - \mu_n| \le \varepsilon_n + C_v \cdot \delta$$

Numerical Example

- **Original Problem:**

$$\frac{d^2 v}{dt^2}(t,Z) + \gamma \frac{dv}{dt} + kv = f\cos(\omega t), \qquad v(0) = v_0, \quad \frac{dv}{dt}(0) = v_1$$

$$Z = (\gamma, k, f, \omega, v_0, v_1) \in \mathbb{R}^6$$

- **Encapsulation Problem:**

$$\frac{d^2 u}{dt^2}(t,X) + X_1 \frac{du}{dt} + X_2 u = X_3 \cos(X_4 t), \qquad u(0) = X_5, \quad \frac{du}{dt}(0) = X_6$$

$$X = (X_1, \ldots, X_6) \in [-1,1]^6$$

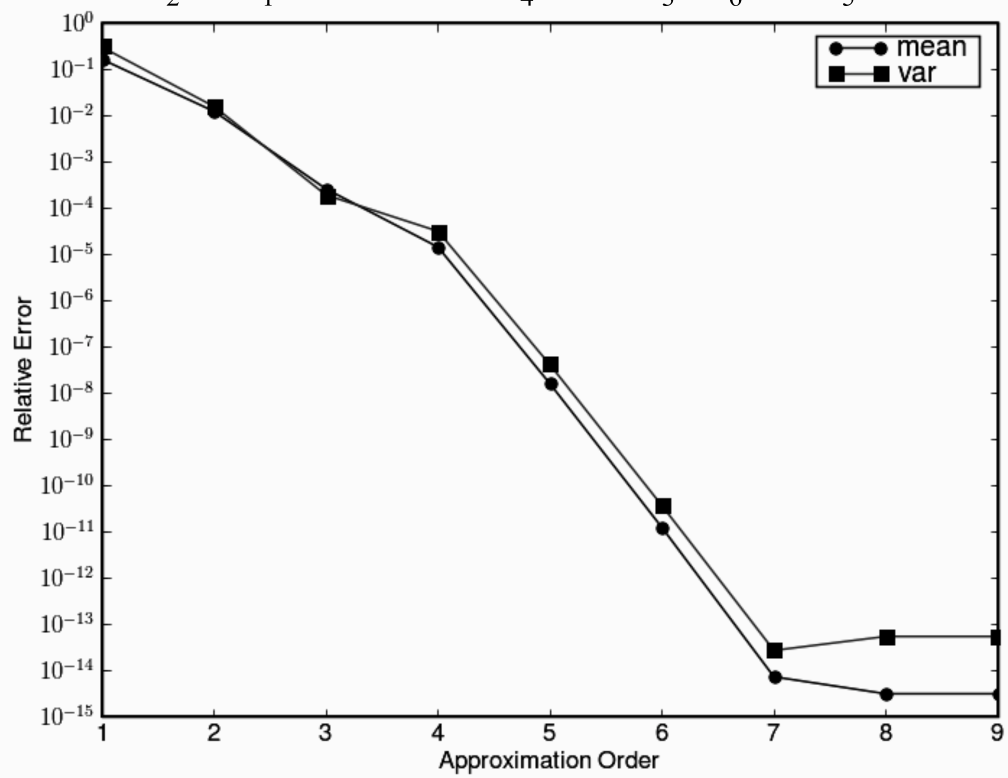
○ Solved by 6-dimensional sparse grid collocation for *t=20*

Dependent Inputs

$$\frac{d^2u}{dt^2}(t,Z) + Z_1\frac{du}{dt} + Z_2 u = Z_3\cos(Z_4 t), \qquad u(0) = Z_5, \quad \frac{du}{dt}(0) = Z_6$$

$Z_1 \sim \text{beta}(0.08,0.12,3,2)$, $Z_3 \sim \text{beta}(0.08,0.1,1,1)$, $Z_5 \sim \text{uniform}(0.45,0.55)$, independent

$$Z_2 = Z_1^2/4 + 0.01,\ Z_4 = 10Z_3,\ Z_6 = (Z_5 - 0.5)$$



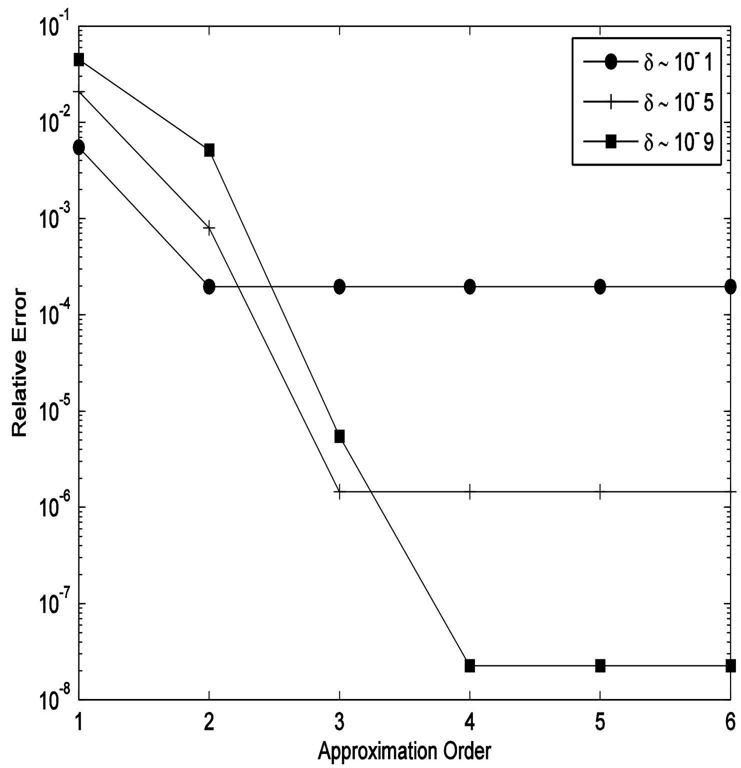
- 4d problem is solved in 6d, without "cutoff"

Unbounded Inputs: Effect of "Cutoff"

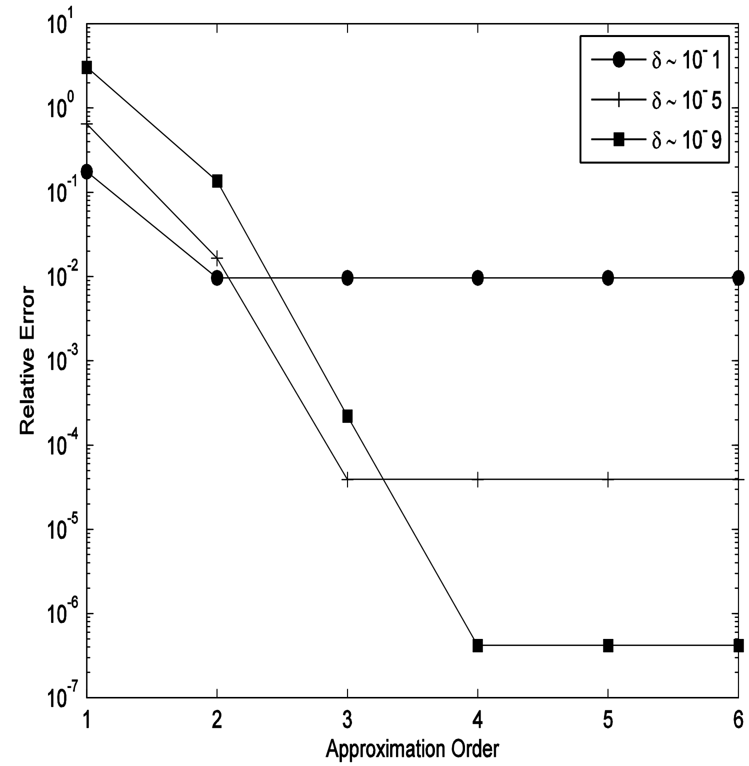
$$\frac{d^2u}{dt^2}(t,Z) + Z_1\frac{du}{dt} + Z_2 u = Z_3\cos(Z_4 t), \qquad u(0) = Z_5, \quad \frac{du}{dt}(0) = Z_6$$

Gaussian: $Z \sim \mathcal{N}(\mathbf{0},\mathbf{C})$, $\quad \mathbf{C} \in \mathbb{R}^{6\times 6}$ is the covariance matrix

$$I_Z = \mathbb{R}^6, \quad I_X = [-a,a]^6, \quad \text{then } \delta > 0$$



Mean

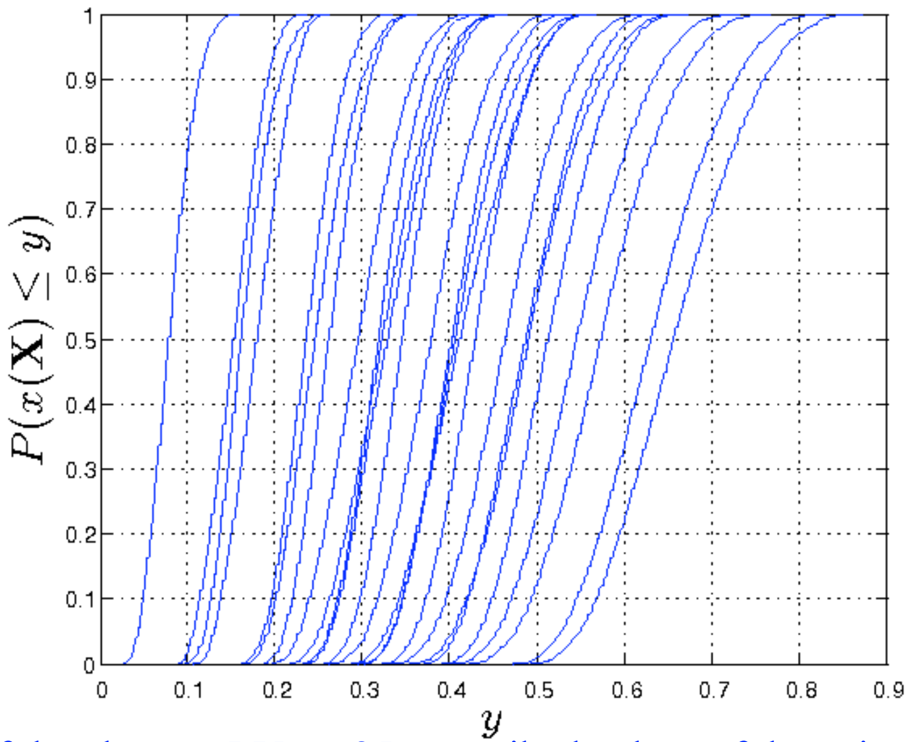


Variance

Mixed Aleatory and Epistemic Case

$$\frac{d^2u}{dt^2}(t,Z) + Z_1 \frac{du}{dt} + Z_2 u = Z_3 \cos(Z_4 t), \qquad u(0) = Z_5, \quad \frac{du}{dt}(0) = Z_6$$

- Aleatory: $Z_1 \sim \text{beta}(0,1,0,0),\ Z_2 = Z_1^2/4 + 0.01, Z_3 \sim \text{beta}(0,1,1,1),\ Z_5 \sim \text{beta}(0,1,2,1)$
- Epistemic: $Z_4 \in [0.8, 1.2], \quad Z_6 \in [-0.05, 0.05]$



CDF of the aleatory RVs at 25 prescribed values of the epistemic variables

- Solution obtained by sparse grid collocation via simultaneous construction (5-d)

Epistemic Uncertainty: Think "Outside the Box"

- **Original Problem:**

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x,Z) = \mathcal{L}(v), & D\times(0,T]\times I_Z \\ \mathcal{B}(v) = 0, & \partial D\times[0,T]\times I_Z \\ v = v_0, & D\times\{t=0\}\times I_Z \end{cases}$$

- **Encapsulation Problem:**

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x,X) = \mathcal{L}(u), & D\times(0,T]\times I_X \\ \mathcal{B}(u) = 0, & \partial D\times[0,T]\times I_X \\ u = v_0, & D\times\{t=0\}\times I_X \end{cases}$$

- **Question: Does I_X have to be a hyber-box?**
  - ✓ **No. I_X can be unbounded too.**
  - ✓ **Numerical solution can converge in L^p norm. (More practical)**
  - ✓ **Additional constraints on the measures are needed.**

Reference:

- J. Jakeman, M. Eldred, D. Xiu, “Numerical Approach for Quantification of Epistemic Uncertainty”, *Journal of Computational Physics, vol. 229*, pp. 4648-4663, 2010.
- X. Chen, E.-J. Park, D. Xiu, Preprint, 2011.

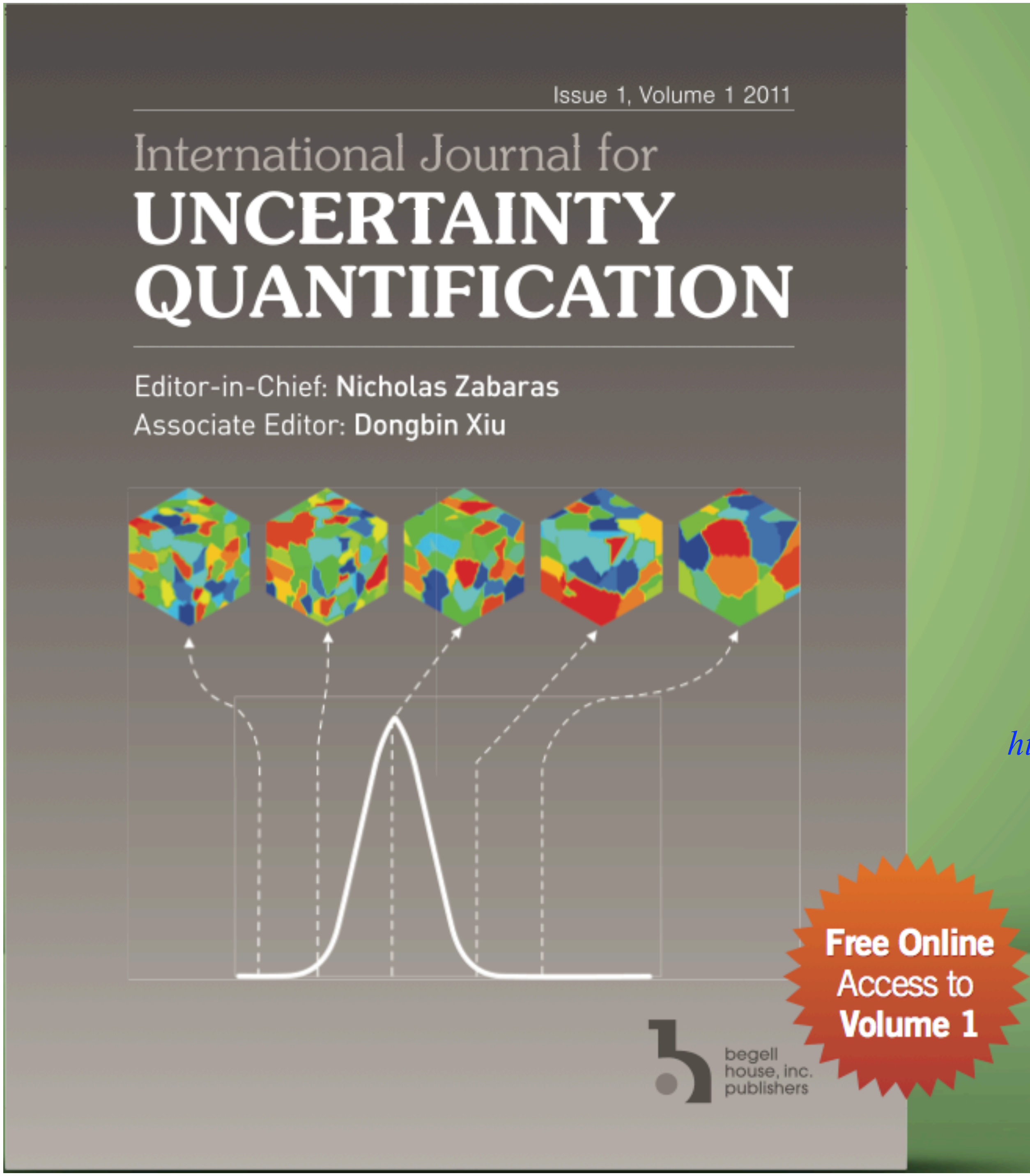
Summary

- Uncertainty Analysis: To provide improved prediction
  - Input characterization
  - Uncertainty propagation
  - Post processing

- Generalized polynomial chaos (gPC)
  - Multivariate approximation theory

- Important directions:
  - Approximation theory in HIGH dimensions
  - Combination with data

- **Data, *any* data, can help**



http://uncertainty-quantification.com/